THE SELECTIVE DEPENDENCE OF THE COLLECTIVE LEVELS IN THE LIGHT NUCLEI (A = 18-80) ON THE J = 0, 2 MATRIX ELEMENTS OF THE EFFECTIVE TWO-BODY INTERACTIONS

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DECLARATION

This is to certify that the work presented in this thesis has been carried out by the candidate under my supervision in the Department of Physics, Indian Institute of Technology, Kanpur, India.

To the best of my knowledge this work is original and has not formed the basis for the awards of any other degree.

S.K. Sharma
1/8/81

Dr. S.K. Sharma
Supervisor

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ABSTRACT

A recent phenomenological model called the "Interacting Boson Model" (IBM) of collective levels in nuclei has been extremely successful in describing the rotational, vibrational as well as transitional nuclei. The IBM treats the lowlying collective states of a system of bosons possessing no intrinsic spin but able to occupy two levels with L=0 and L=2. We have presented Hartree-Fock calculations, employing realistic interactions for several nuclei in the 1s-0d, 1p-0f and 1p-0f-0g shells with a view to examine some of the assumptions implicit in the formulation of the IBM.

CONTENTS

CHAPTER I

INTRODUCTION

Nuclear Many-body Problem: Simple Shell Model and Configuration Mixing:-

There is hardly a single worthwhile problem with realistic interactions in quantum mechanics which can be exactly solved for a many particle system. However approximate solutions based on intuition have been of valuable help. An outstanding example of this is provided by the well-known atomic Hartree method.

The success of the atomic Hartree method led the early nuclear physicists to believe that within a nucleus also an individual nucleon moves in some average potential produced by all other nucleons.[11] In this way the shell model of the nucleus evolved and after that the shell model has gone through various stages of development.

The average potential stated above can be taken to be either an infinitely deep square-well or a harmonic oscillator potential. For both these potentials Schrodinger's equation can be solved exactly and we get various energy levels. In the single particle model, the nucleus is visualised to consist of filled shells consisting of maximum number of neutrons and protons permitted by the Pauli's exclusion principle as well as partially filled shells. This model is very simple in the sense that the nuclear properties are characterised by the last unpaired

nucleon. In an even-even nucleus all the nucleons are paired and so the spin of the nucleus is zero. In the case of odd-even nucleus the spin is given by the last unpaired nucleon and in the case of odd-odd nucleus the spin is given by the unpaired neutron and proton. In the early stage of development of nuclear shell model one of the main objective was to explain the magic numbers. There are very strong experimental evidences that when a nucleus contains 2,8,20,50,82 or 126 protons or neutrons a shell closure occurs.[12] These numbers are called magic numbers. Let us see how the various stages of nuclear shell model could explain the magic numbers and other electromagnetic and nuclear properties of the ground state.

The eigenstates are obtained in a spherically symmetric potential v(r) by solving the Schridinger's equation,

$$\left[\nabla^2 + \frac{2M}{\hbar^2}\left(E - v(r)\right)\right]\psi(\vec{r}) = 0 \qquad \text{(I.1)}$$

The solution of this equation is of the type

$$\psi_{nlm}(\vec{r}) = U_{nl}(r)\, Y_{lm}(\theta,\phi) \qquad \text{(I.2)}$$

In the case of infinite depth square well the radial wavefunction is given by the spherical Bessel functions which are regular at the origin

So, in this case,

$$U_{nl}(r) = j_l(kr) \qquad \text{(I.3)}$$

From the boundary condition $j_l(kR) = 0$ where R is the radius of the square well, we get the energy eigenvalues. It is seen that the level l is 2(2l+1) fold degenerate.

The closed shells occur for neutron and proton numbers $\sum_{l} 2(2l+1)$ with $l = 0,1,2,..$ i.e., at numbers, 2,8,18,20,34, 40,58,68,70,92,106,112,138,156. So, we see that the infinite-depth square well can explain the magic numbers 2,8,20 but the magic numbers 28,50,82 and 126 are not reproduced by the square well.

If we take harmonic oscillator potential then the radial wavefunction is given by[12]

$$U_{nl}(r) = \frac{R_{nl}(r)}{r}, \text{ where,}$$

$$R_{nl}(r) = N_{nl} \exp\left(-\tfrac{1}{2}\alpha r^2\right) r^{l+1} \xi_{nl}(r) \quad \cdots \quad (1.4)$$

$$\xi_{nl}(r) = L^{l+1/2}_{n-l-1/2}(2\alpha r^2)$$ which is the Laguerre Polynomial and N_{nl} is a normalisation constant. The energy levels are given by

$$E_{nl} = \hbar\omega\,(2n+l-1/2) \quad \cdots \quad (1.5)$$

$n = 1,2,3,..$ $l = 0,1,2,..$

The levels appear in the sequence of groups 1s;1p; 1d,2s; 1f,2p; 1g,2d; 3s,etc. The closed shells occur at

2,8,20,40,70,112,168

So, the harmonic oscillator potential also explains the magic numbers 2,8,20 but not the higher ones.

Therefore we see that both the square well and the harmonic oscillator potential cannot explain the magic numbers beyond 20. To obtain the magic numbers 28,50,82, 126, Mayer, Haxel Jensen and Suess suggested that a spin

orbit potential $-f(r)\ (\bar{l}.\bar{s})$ should be added to the centrally symmetric potential. This results in the splitting of $j = l \pm \frac{1}{2}$ levels. (s is the intrinsic spin of the nucleon) The choice of the sign in the potential is such that $j=l+\frac{1}{2}$ level is depressed relative to the $j = l - \frac{1}{2}$ level. This explains all magic mumbers viz., 2,8,20,28,50,82,126. The infinite range harmonic oscillator potential can be brought closer to the finite square well if we cut off the range after a finite value. This can ~~be~~ effectively be achieved by adding a $\alpha\rho^2$ term to the potential. Here α is negative. So, after this development the complete hamiltonian of a single necleon in a spherically symmetric potential is given by

$$H_i = t_i + \frac{1}{2}m\omega^2 r_i^2 + \alpha \vec{l}_i \cdot \vec{l}_i + \beta \vec{l}_i \cdot \vec{s}_i \quad \cdots\cdots (I\,6)$$

The spin-orbit splitting term has a relativistic orgin.

Actually a potential which is intermediate between the square-well and the harmonic oscillator well and which also has an experimental basis, is the Wood Saxon potential obtained by fitting the data on nucleon-nucleon scattering. This potential which is flat at the centre, and falls off smoothly to zero at the edge of the nucleus is given by (12)

$$V(r) = -V_0 \left[1 + \exp \mu (r - R)\right] \quad \cdots\cdots (I\,7)$$

where $\mu^{-1} \simeq 0.5 \times 10^{-13}$cm and $R \simeq 1.33A^{\frac{1}{2}} \times 10^{-13}$ cm, A being the mass number of the nucleus and $V_0 \simeq$ 50-60 Mev.

The single-particle model described above explains not only the magic numbers but the spin and parity of a large

number of nuclei, provided we make the following assumptions.(11)

1. Even-even nuclei, that is, nuclei with even Z and even N have total ground state angular momentum $J = 0^+$.

2. An odd nucleus, that is, a nucleus with odd Z or odd N, will have a total ground state angular momentum and parity equal to the half-integral angular momentum j and the parity $(-1)^l$ of the unpaired particle.

3. An odd-odd nucleus will have a total angular momentum which is the vector sum of the odd neutron and odd proton J values.

$$J = j_p + j_n.$$

The quantum number J is therefore an integer between the limits

$$|j_n - j_p| \leq J \leq |j_n + j_p|$$

The parity will be the product of the proton and neutron parity that is, $= (-1)^{l_n + l_p}$.

A partial justification for the above assumption arises from the tendency of the nucleon-nucleon interaction to give a J = 0 pair for two particles in (jm), (j-m) states.

Although the simple, shell model predicts successfully the ground state spin and parity for many nuclei, it fails to give the ground state magnetic moment correctly. It can only give the limits between which the experimental depole moments lie. The two limits of the dipole moment when there is an unpaired nucleon in an odd-A nucleus, are

$$\mu = \tfrac{1}{2} g_s + \left(J - \tfrac{1}{2}\right) g_l \qquad \text{when} \quad J = l + \tfrac{1}{2}$$

$$\mu = \frac{1}{J+1}\left[-\tfrac{1}{2} g_s + \left(J + \tfrac{3}{2}\right) g_l\right] \qquad \text{when } J = l - \tfrac{1}{2}.$$

where g_s and g_l are the g-factors for the spin and orbital motion.[11]

The discrepancy between the experimental result and the calculated value of magnetic moment suggests that the simple shell model is not perfectly alright. The main drawback of the shell model is that there we have assumed a spherically symmetric potential of the nucleus, whereas, in reality most of the nuclei are deformed. The assumption of spherical symmetry is valid only in the immediate neighbourhood of a closed shell and when the quadrupole moment is zero. In the case of a nucleus where the number of particles are such as to be in between two shells, the spherial symmetry is lost and the quadrupole moment has appreciable value.

Due to the incorrect assumption of spherical symmetry in the shell model the nuclear state is not given by the eigenstate of last unpaired nucleon, as the shell model predicts. Rather, the eigenstate may be the linear combination of shell model eigenstates, and this eigenstate will represent a deformed nucleus.

When there are a number of nucleons in a partially filled shell, outside a filled core, the nucleons can be in various configuration due to the residual interaction

between nucleon pairs. So the nuclear eigenstate will be the linear combination of the eigenstates of various configurations for a particular total angular momentum. This is called configuration mixing. By considering configuration mixing we can calculate exactly the low-lying nuclear energy levels and the corresponding eigenfunctions. To illustrate the configuration mixing calculation, let us take the example of oxygen 18. It has two neutrons outside the closed core of 16. These two neutrons can be in any of the three states $0d_{5/2}$, $1s_{1/2}$, $0d_{3/2}$. If we want to calculate the nuclear eigenstate corresponding to J = 0 we have to consider the case when the neutrons are in the same j state. So the configurations will be $|(0d_{5/2})^2\rangle_{J=0}$ $|(1s_{1/2})^2\rangle_{J=0}$ and $|(0d_{3/2})^2\rangle_{J=0}$. The nuclear eigenstate will be the linear combination of these states. The coefficients are obtained by diagonalising the matrix having matrix element of the type $\langle |V| \rangle$ where V is the two-body interaction.

But, judging from the practical point of view , configuration mixing calculations can be done only for low-lying states of the nuclei and only when the configuration space is small. If we want to calculate the nuclear eigenstate for a high angular momenta or in a large configuration space (i.e., in the case of heavy nuclei), the size of the matrix we have to diagonalise becomes enormously

large and prevents us to proceed further. We have however, a better alternative which is the deformed Hartree-Fock self-consistent method. As yet the Hartree-Fock self-consistent method is known to be the most satisfactory approximate nuclear many-body technique for all sorts of nuclei where shell model calculations become impracticable.

CHAPTER II

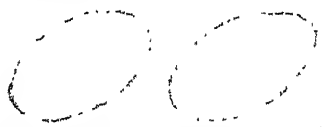
II.1 Hartree-Fock Method as the best Zeroth-order treatment of the nuclear many-body problem :

So, the Hartree-Fock method essentially is a many-body technique of finding out approximate nuclear eigenstates Nowadays, two many body techniques are available in physics, broadly speaking. (i) Canonical transformation approach (ii) Quantum field theoretic propagator approach. In canonical transformation approach the interacting system is transformed into a nearly nonintracting system. In this way we can get two types of excitations.

(i) Collective excitations (e.g., phonons in solid)

(ii) Quasiparticle excitation (e.g., nuclei etc.).In collective excitation we talk of the excitation of the system as a whole and in quasiparticle excitation we concentrate on a single particle surrounded by the cloud of other kind of particles. The quasiparticles are almost non-interacting. We can naively say that the Hartree-Fock method is a kind of many-body technique which falls in the category of quasiparticle excitation . Here we talk about the individual orbits but the orbits are noninteracting and deformed. The basic scheme is as follows:

Undeformed orbits with interaction



Deformed orbits with reduced interaction

We go from the undeformed orbits with interaction to deformed orbits with reduced interaction, which is then neglected in the first approximation. Here, unlike the canonical transformation, we do not have to find out the eigenstate of deformed orbits by any transformation. We can immediately write down the hamiltonian of the deformed orbits since the deformation is quadrupole type. The HF selfconsistent deformed orbits can also be interpreted, at a phenomenological level, in terms of the eigenstates of the Nilsson hamiltonian

$$h = h_0 + \chi \vec{l}\cdot\vec{s} + \rho \vec{l}^2 + \delta Y_0^2 \qquad \text{(II 1.1)}$$

The last term in the above expression contains the spherical harmonic Y_0^2 which takes into account the quadrupole deformation. This hamiltonian is suitable when we deal with axial Hartree-Fock method, where the projection of the total angular momentum on the z-axis of the intrinsic frame of reference has a good quantum number. It should be mentioned here that deformations of most of the nuclear orbits are of quadrupole type.

It is seen that when there is a number of nucleons outside a core of filled shells, the lowlying nuclear eigenstates are quasi-rotational type. The levels are not found to be exactly rotational in the sense that the energies of the various angular momentum levels are not exactly proportional to J(J+1) but there is another term

which is proportional to $J^2(J+1)^2$, but whose coefficient is small. Actually, the total nuclear eigenstate can be written as the product of intrinsic wavefonction and rotational wavefunction. This is called Bohr-Mottelson's unified model. In this model e.g., the state of spin J belonging to the ground state rotational band of an even-even nucleus is described by the wavefunction[1]

$$|JM\rangle = \sqrt{\frac{2J+1}{8\pi^2}}\, D^{J*}_{M0}(\Omega)\,|\phi_k\rangle \qquad J = 0, 2, 4 \qquad (II.12)$$

The rotational motion is described by the symmetric top wavefunction

$$D^{J*}_{M0}(\Omega) = \sqrt{\frac{4\pi}{2J+1}}\, Y^J_M(\beta,\gamma) \qquad (II.13)$$

The intrinsic state $|\phi_k\rangle$ is in the form of antisymmetric slater determinant containing the eigenstates of deformed orbits. The deformed orbits are given by the eigenstate of the Nilsson hamiltonian h.

$$h|\lambda\rangle = e_\lambda|\lambda\rangle \qquad (II.14)$$

We'll be dealing with the nucleons in the single major shell outside the closed core. This type of restrictive outlook has the justification that the energy difference between two major sheels is high enough to neglect the interaction between two major shells in comparison to the interaction between the nuclei within the same major shell.

It is the task of Hartree-Fock method to determine the deformed orbits $|\lambda\rangle$. This is done by a variational method given below. In this method we minimise the ground state

energy of the nucleus, which is the expectation value of the nuclear hamiltonian H in the Hartree-Fock states

The nuclear hamiltonian H and the Hartree-Fock energy are given by

$$H = \sum_{i=1}^{A} \frac{p_i^2}{2m} - \frac{1}{2}\sum_{i\neq j} v(ij) \qquad \text{(II.15)}$$

and

$$E_{HF} = \langle \Phi | H | \Phi \rangle = \sum_{\lambda=1}^{A} \langle \lambda | t | \lambda \rangle + \frac{1}{2}\sum_{\lambda,\mu=1}^{A} \langle \lambda\mu | v | \lambda\mu \rangle \qquad \text{(II.16)}$$

respectively.

$\langle \lambda | t | \lambda \rangle$ is the kinetic energy of the orbit λ and $\langle \lambda\mu | v | \lambda\mu \rangle = -\langle \lambda\mu | v | \mu\lambda \rangle$ is an antisymmetrised matrix element of the two-body interaction v(ij).

It is advantageous to expand the orbits on a basis of known wavefunction.

$$|\lambda\rangle = \sum_j C_j^{\lambda} |j\rangle \qquad \text{(II.17)}$$

The basis j may be e.g., the set of $|n\ell jm\tau\rangle$ of shell model states in a harmonic oscillator well. Any basis may be used to expand the orbits provided one is able to calculate the matrix elements of the interaction v with the basis states. The set of orbits $|\lambda\rangle$ (both filled and unfilled) is assumed to form a set of orthonormal set of wavefunctions.

$$\sum_j C_j^{\lambda *} C_j^{\lambda'} = \delta_{\lambda\lambda'}$$
$$\sum_{\lambda} C_j^{\lambda *} C_{j'}^{\lambda} = \delta_{jj'} \qquad \text{(II.18)}$$

The wavefunction $|\Phi\rangle$ is determined by the coefficients C_j^λ which become variational parameters. The energy will be stationary with the above normalisation condition when

$$\frac{\partial}{\partial C_j^{\lambda *}}\left[\langle\Phi|H|\Phi\rangle - \epsilon_\lambda \sum_j C_j^{\lambda *} C_j^\lambda\right] = 0 \quad \cdots\cdots (II.9)$$

Here ϵ_λ is introduced as a Lagrange multiplier. With the help of the expansion of λ, the above equation may be expressed in terms of known matrix elements of t and v in the known basis j. The derivative may then be calculated directly, and one obtains

$$\sum_{j'}\left[\langle j|t|j'\rangle + \sum_{\lambda=1}^{A}\sum_{j_1 j_2} C_{j_1}^{\lambda *}\langle j j_1|v|j' j_2\rangle C_{j_2}^\lambda\right] C_{j'}^\lambda = \epsilon_\lambda C_j^\lambda \quad \cdots\cdots (II.1.10)$$

This equation has the form of that of an eigenvalue problem

$$\sum_{j'}\langle j|h|j'\rangle C_{j'}^\lambda = \epsilon_\lambda C_j^\lambda \quad \cdots (II.1.11)$$

where h is the hamiltonian given by the matrix elements

$$\langle j|h|j'\rangle = \langle j|t|j'\rangle + \sum_{\lambda=1}^{A}\langle j\lambda|v|j'\lambda\rangle$$

$$= \langle j|t|j'\rangle + \sum_{\lambda=1}^{A}\sum_{j_1 j_2} C_{j_1}^{\lambda *}\langle j j_1|v|j' j_2\rangle C_{j_2}^\lambda \quad \cdots (II.1.12)$$

h is the Hartree-Fock hamiltonian. The coefficients C_j^λ's are obtained from the above equation by a self-consistent iterative method which is as follows:[1]

(i) An initial set of values of the coefficients are taken.

(ii) By these set of values the matrix elements of h are calculated from the equation (Eq. 1.12)

(iii) The matrix is diagonalised and a new set of coefficients C_i^{λ} are obtained.

(iv) These new set of coefficients are utilised to calculate the matrix element and we back to step (ii)

In this way the iteration is continued until the coefficients in two successive iterations differ very little from each other. At every stage of iteration we can calculate also the Hartree-Fock energy E_{HF} and compare its value in successive iterations.

The choice of initial guess in Hartree-Fock iteration is very crucial because different types of initial guess lead to different Hartree-Fock minima.

To get the rotational intrinsic Hartree-Fock state it is best to generate the initial guesses from the quadrupole operator i.e., we can generate the C_i^{λ}'s by diagonalising the matrix of quadrupole operator.(1)

From the axial Hartree-Fock method we can know the eigenstate of J_z and the corresponding energy. That is, we can know some sort of average energy, and average wavefunction. Each value of total angular momentum projection corresponds to a rotational band.

II.2 Angular Momentum Projection (1.7.18)

From the Hartree-Fock wavefunction, the nuclear eigenfunctions of (J^2, J_z) can be obtained by angular momentum projection technique.

Let us write $\psi_{K=0}(H.F.) = \sum_J A_J \psi_{JK}$ ... (II 2.1)

where $\psi_{K=0}(HF)$ is the Hartree-Fock wavefunction for the K=0 band. Here, we are expanding the average wavefunction obtained in Hartree-Fock method in terms of eigenstates of J^2 and J_z.

To find $|A_J|^2$, let us consider,

$$e^{-i\beta J_y}\psi_{K=0} = \sum_J A_J e^{-i\beta J_y}\psi_{JK} \quad \text{... (II 2.2)}$$
$$= \sum_J A_J \sum_{K'} d^J_{KK'}(\beta)\psi_{JK'}$$

where $e^{-i\beta J_y}$ is a rotation operator around the 2-axis and $d^J_{KK'}$ is the d-matrix. β is the angle of rotation.

Thus, we get

$$\langle\psi_{K=0}|e^{-i\beta J_y}|\psi_{K=0}\rangle$$
$$= \sum_{J'} A^*_{J'} \sum_J A_J \sum_{K'} d^J_{KK'}(\beta)\langle J'K|JK'\rangle \quad \text{(II.2.3)}$$

From this we can get A's as

$$\int_0^{\pi/2} \langle\psi_{K=0}|e^{-i\beta J_y}|\psi_{K=0}\rangle d^{J''}_{KK}(\beta)d\Omega = |A_{J''}|^2 \quad \text{... (II.2.4)}$$

A technique to calculate $\langle \Psi_{K=0} | e^{-i\beta J_y} | \Psi_{K=0} \rangle$ is as follows. We can construct

$$\langle \Psi_{K=0} | e^{-i\beta J_y} | \Psi_{K=0} \rangle$$

$$= \langle |\phi| \quad | \quad |\tilde{\phi}| \rangle$$

unrotated determinant — rotated determinant

For example, let us consider the case of 2x2 determinant

$$e^{-i\beta \hat{j}_y(1)} e^{-i\beta \hat{j}_y(2)} \begin{vmatrix} \phi_{K=\frac{1}{2}}(1) & \phi_{K=\frac{1}{2}}(2) \\ \phi_{K=-\frac{1}{2}}(1) & \phi_{K=-\frac{1}{2}}(2) \end{vmatrix}$$

$$= \begin{vmatrix} \tilde{\phi}_{K=\frac{1}{2}}(1) & \tilde{\phi}_{K=-\frac{1}{2}}(2) \\ \tilde{\phi}_{K=-\frac{1}{2}}(1) & \tilde{\phi}_{K=\frac{1}{2}}(2) \end{vmatrix} \quad \cdots \quad (\text{II}.2.6)$$

where $\tilde{\phi}_{K=\frac{1}{2}}(1) = e^{-i\beta \hat{j}_y(1)} \phi_{K=\frac{1}{2}}(1)$

$$= e^{-i\beta \hat{j}_y(1)} \sum_K C_K^j \phi_{jK}(1,2)$$

$$= \sum_K C_K^j \sum_{K'} d^j_{KK'}(\beta) \phi_{jK'}$$

So, $\langle |\phi_1| \, | \tilde{\phi}_1| \rangle = \begin{vmatrix} \langle \phi_1^1 | \tilde{\phi}_1 \rangle & \cdots \\ \cdots & \cdots \end{vmatrix}$

where,

$$\langle \phi_1 | \tilde{\phi}_1 \rangle = \left\langle \sum_{j''} C_K^{j''} \phi_K^{j''} \middle| \sum_{j'} C_K^{j'} \sum_{K'} d^{j'}_{KK'}(\beta) \phi_{j'K'} \right\rangle$$

$$= \sum_{j'} |C_K^{j'}|^2 \sum_{K'} d^{j'}_{K'K}(\beta) \quad \cdots \quad (\text{II}.2.7)$$

The energies corresponding to different J's can be obtained as follows

$$\langle \psi_{K=0} | H | \psi_{K=0} \rangle = \sum_J |A_J|^2 E_J \quad \cdots (II\ 2.8)$$

where $E_J \equiv \langle \Phi^J_{JK} | H | \Phi^J_{JK} \rangle$

In equation (II.2.4) we have obtained,

$$|A_J|^2 = 2 \int_0^{\pi/2} \langle \psi_{K=0} | e^{-i\beta J_y} | \psi_{K=0} \rangle d^J_{00}(\beta) d\Omega \quad \cdots (II\ 2.9)$$

In a similar manner, we can get,

$$E_J |A_J|^2 = 2 \int_0^{\pi/2} \langle \psi_{K=0} | e^{-i\beta J_y} H | \psi_{K=0} \rangle d^J_{00}(\beta) d\Omega$$

$$\therefore E_J = \frac{\int_0^{\pi/2} \langle \psi_{K=0} | e^{-i\beta J_y} H | \psi_{K=0} \rangle d^J_{00}(\beta) d\Omega}{\int_0^{\pi/2} \langle \psi_{K=0} | e^{-i\beta J_y} | \psi_{K=0} \rangle d^J_{00}(\beta) d\Omega} \quad \cdots (II.2.10)$$

By this formula, the energy corresponding to each J in a band is determined.

II.3 The interacting boson model and investigation of the validity of its basic assumption in the framework of HF method:-

Attempts have been made at various stages to develope a truncation scheme for the large configuration space of shell model, so that shell model calculations become practicable for medium and heavy-mass nuclei.(8) But such a truncation schemes have not yet been completely successful.

Recently a much simplified model has come into picture, which can successfully reproduce the collective behaviour of nuclei, specially the medium and heavy-mass nuclei. This model is called Interacting Boson Model. The central idea of this model is this: The Fermion system of the nucleons is grouped into pairs which are bosons. The collective behaviour of the nuclei depends only on the bosons having spins 0 and 2 i.e., the s-bosons and d-bosons.[10,16] The s-bosons and d-bosons interact among each other to form the multiparticle system. The Hamiltonians of interacting boson model are found in literature and such Hamiltonians have analytic solutions for energy spectra etc. But derivation of interacting boson model from shell model i.e., the microscopic description of the model has not yet been developed with much success. So, why the collective behaviour depends selectively on two particle states of angular momenta 0 and 2 only, is not yet known.[10]

Hartree-Fock method was developed to do away with the difficulties connected with shell-model calculations, and here we do not need any truncation scheme for simplification. But the basic assumption of interacting boson model can easily be judged in the frame-work of HF calculations by switching off the two body interactions when their total angular momentum is other than 0 or 2 . We have found that the qualitative features of low-lying

spectra remain unchanged when we go from full interaction to selective interaction, involving two-particle states having angular momenta 0 and 2 only. Thus the basic assumption of the interacting boson model is justified.

CHAPTER III

CALCULATIONAL PROCEDURES

We have described the Hartree-Fock equations and angular momentum projection in Chapter II. Now we'll briefly describe the calculational procedure alongwith the techniques involved in computer programming.

III.1 Storage of two-body matrix elements:-

We have used matrix elements of Kuo -Brown realistic interaction[22] available in literature. The two-body matrix elements of the form $\langle j_1 j_2 | V | j_3 j_4 \rangle_{JT}$ are stored in a three-dimensional array in the program, for easy reference. There is a special indexing procedure for this. Let us illustrate this indexing procedure taking the example of the s-d shell. In the s-d shell space, $(0d_{5/2}, 1s_{1/2}, 0d_{3/2})$ We have three angular momenta which we can index as 1,2,3. Now, j_1, j_2 on the bra-side of the matrix element can be indexed as

$$n_1 = 3(j_1-1) + j_2 \qquad \text{(III.1.1)}$$

when j_1 and j_2 varies from 1 to 3,

n_1 varies from 1 to 9.

Similarly j_3, j_4 on the ket side can be indexed as

$$n_2 = 3(j_3-1) + j_4 \qquad \text{(III.1.2)}$$

For JT, we have $n_3 = 2J + T$ (III.1.3)

when $J = 0$, $T = 1$, $n_3 = 1$

$J = 1$ $T = 0$ $n_3 = 2$ and so on.

In s-d shell n_1 can run from 1 to 9, n_2 from 1 to 9 and n_3 from 1 to 10.

By this indexing procedure, also it is easy to incorporate the symmetry properties of the matrix elements. The matrix-elements have the following symmetry properties.

$$\langle j_2 j_1 | V | j_3 j_4 \rangle_{JT} = \langle j_1 j_2 | V | j_3 j_4 \rangle_{JT} \times (-1)^{j_1+j_2+J+T}$$

$$\langle j_3 j_4 | V | j_2 j_1 \rangle_{JT} = \langle j_2 j_1 | V | j_3 j_4 \rangle_{JT}$$

$$\langle j_1 j_2 | V | j_4 j_3 \rangle_{JT} = \langle j_1 j_2 | V | j_3 j_4 \rangle_{JT} \times (-1)^{j_3+j_4+J+T}$$

$$\langle j_4 j_3 | V | j_1 j_2 \rangle_{JT} = \langle j_1 j_2 | V | j_4 j_3 \rangle_{JT}$$

$$\langle j_2 j_1 | V | j_4 j_3 \rangle_{JT} = \langle j_1 j_2 | V | j_3 j_4 \rangle_{JT} \times (-1)^{j_1+j_2+j_3+j_4}$$

$$\langle j_4 j_3 | V | j_2 j_1 \rangle_{JT} = \langle j_2 j_1 | V | j_4 j_3 \rangle_{JT} \quad \text{---(III.1.3)}$$

III.2 Definition of the basis

The basis in which the deformed orbital of the nucleon is expanded should be such that the expansion converges and the matrix elements of two-body interaction in such basis are readily available. The harmonic oscillator wavefunction shows good convergence and in shell model basis the matrix elements are available. We have chosen the basis such that they are suitable for non-axial as well as axial Hartree-Fock calculation.

In axial Hartree-Fock calculation, the deformed orbital will be an eigenstate of j_z , the projection of angular momentum.

The basis chosen in different shells are given below:-

sd-shell:- $0d_{5/2}, 1/2$; $0d_{3/2,1/2}$; $1s_{1/2,1/2}$; $0d_{5/2,3/2}$; $0d_{3/2,3/2}$; $0d_{5/2,5/2}$

We have taken experimental single-particle energy of oxygen-17

Orbit	Energy (Mev)
$0d_{5/2}$	0
$1s_{1/2}$	0.87
$0d_{3/2}$	5.08

f-p shell:-

The basis is

$f_{7/2,1/2}$; $f_{5/2,1/2}$; $p_{3/2,1/2}$; $p_{1/2,1/2}$; $f_{7/2,3/2}$; $f_{5/2,3/2}$;

$p_{3/2,3/2}$; $f_{7/2,5/2}$; $f_{5/2,5/2}$, $f_{7/2,7/2}$

Single particle energies:-	Orbits	Energy (Mev)
	$0f_{5/2}$	6.25
	$1p_{1/2}$	3.9
	$1p_{3/2}$	2.1
	$0f_{7/2}$	0.0

f-p-g shell: - The basis is

$0g_{9/2,9/2}$; $0g_{9/2,5/2}$; $0f_{5/2,5/2}$; $0g_{9/2,1/2}$; $0f_{5/2,1/2}$;

$1p_{3/2,1/2}$; $0g_{9/2,-3/2}$; $0f_{5/2,-3/2}$; $1p_{9/2,-3/2}$; $0g_{9/2,-7/2}$

Single particle energies:-	Orbits	Energies (Mev)
	$1p_{3/2}$	0.0
	$0f_{5/2}$	0.78
	$1p_{1/2}$	1.05
	$0g_{9/2}$	3.25

III.3 Storage of Clebsch Gordan coefficients:-

For storing all sorts of Clebsch-Gordan Coefficient, we use the indexing procedure,

$$n_1 = (j_1+1/2)^2 + m_1 + 1/2$$
$$n_2 = (j_2+1/2)^2 + m_2 + 1/2 \qquad \text{(III.2.1)}$$

Let us see how n_1 goes,

when, $j_1 = 1/2 \quad m_1 = -1/2 \qquad n_1 = 1$

$j_1 = 1/2 \quad m_1 = 1/2 \qquad n_1 = 2$

$j_1 = 3/2 \quad m_1 = -3/2 \qquad n_1 = 3$ and so on.

Similarly for j_2.

The Clebsch-Gordan coefficients are again stored as a three-dimensional array of numbers; viz., CLBGD (n_1, n_2, J) where J is the total angular momentum. The Clebsch-Gordan coefficients are generated by a subroutine called THREEJ

III.4 Generation of trial wavefunction to start Hartree-Fock iteration.

We generate the trial wavefunctions of the HF iteration by diagonelising the matrix of a quadrupole operator, since the deformation of nucleon orbits are quadrupole type. In (nljm) harmonic oscillator basis, the matrix element of quadrupole operator

$$Q_0^2 \quad \left(= \frac{16}{5} r^2 y_0^2 \right)$$

may be written as

$$\left\langle n'l'j'm' \middle| Q_0^2 \middle| nljm \right\rangle = (-1)^{j'+1/2} \sqrt{\frac{16\pi}{5}} \left[\frac{(2j+1)(2j'+1)5}{4} \right]^{1/2} \begin{pmatrix} j' & 2 & j \\ 1/2 & 0 & -1/2 \end{pmatrix} \begin{pmatrix} j' & 2 & j \\ m' & 0 & m \end{pmatrix} \left\langle n'l' \middle| r^2 \middle| nl \right\rangle \quad \text{-(III.4.1)}$$

$\left\langle n'l' \middle| r^2 \middle| nl \right\rangle$ can be easily evaluated utilising the

property of harmonic oscillator hamiltonian and so we can write the matrix element above as the product of two Clebsch-Gordan coefficients and a constant . The matrix to be diagonalised is completed by adding the single-particle energies to the diagonal elements. The diagonalisation and finding out the corresponding eigenvectors are done by a subroutine called EIGEN.

III.5 The Hartree-Fock iteration.

The HF iteration is done by comparing the HF energy E_{HF} at every stage of iteration. E_{HF} is calculated with the HF wavefunctions at every stage of iteration. The Hartree-Fock energy and the quadrupole deformation parameter are computed by a subroutine called QERG. At each stage of iteration the summation $\sum_{\lambda} C^{j\lambda}_{j_1} C^{\lambda}_{\cdot\cdot}$ is computed by a function RHO.

III.6 Degeneracies of HF wavefunction.

If for a particular occupied orbit $|\lambda\rangle$, the orbit $|\bar{\lambda}\rangle = e^{-i\pi J_y}|\lambda\rangle$ is also occupied then the HF hamiltonian is said to have time reversal symmetry. An orbit is degenerate with its time-reversed orbit.

In even-even nuclei, time-reversal symmetry is obtained by requiring that, for each occupied orbit,

$$|\lambda\rangle = \sum_{nljm} C^{\lambda}_{nljm} |nljm\,\tau_\lambda\rangle \quad \text{- - - -} \quad \text{(III.6.1)}$$

the time-reversed orbit

$$|\bar{\lambda}\rangle = T|\lambda\rangle = \sum_{n\ell j m} C^{\lambda^*}_{n\ell j m}(-1)^{\ell+j-m}\,|n\ell j -m\rangle \qquad \text{(III.6.2)}$$

is also occupied and orthogonal to $|\lambda\rangle$.

If a nucleus contains equal number of protons and neutrons outside a core then we can fill the same orbit $|\lambda\rangle$ with a neutron and a proton. Then the HF hamilonian is said to have isopin invariance. In this case the neutron and proton orbits are degenerate. In an even-even nucleus, if for each occupied orbit the time reversed orbit is also filled then the HF wavefunctions have four-fold degeneracy.

III.7 Angular Momentum projection[6]:-

We'll briefly outline the angular momentum projection technique here which is actually much more involved. There is well-established technique of angular momentum projection based on the framework of Hartree-Fock Bogoliubov (HFB) theory[4,5] where the orbits are assigned fractional occupation ~~and~~ probabilities (between 0 and 1) unlike in the case of pure Hartree-Fock theory where the occupied orbits have occupation probability one and others zero

The intrinsic deformed state in the HFB theory is given by

$$|\phi_0\rangle = \prod_{im}\left(u_i^m + v_i^m b_{im}^\dagger b_{i\bar{m}}^\dagger\right)|0\rangle$$

where the amplitudes u_i^m and v_i^m characterise the emptiness and fullness[9] respectively of the orbit im. When $u_i^m = 0$ and $v_i^m = 1$ we get pure HF case. $|0\rangle$ is the true vacuum of the nucleus.

The creation operators are expanded in terms of those in the shell model spherical well i.e.

$$b^{+}_{JM} = \sum_{j} C^{jm}_{j,\frac{1}{2},M} a^{+}_{jm} \qquad b^{+}_{J\bar{m}} = \sum_{j} (-1)^{j-m} C^{jm}_{j,\frac{1}{2},M} a^{+}_{j-m} \qquad (III.7.2)$$

The wavefunction (III.7.1) can be written as

$$|\phi_0\rangle = N \exp\left(\frac{1}{2}\sum_{\alpha\beta} f_{\alpha\beta} a^{+}_{\alpha} a^{+}_{\beta}\right)|0\rangle \qquad (III.7.3)$$

Where $$f_{\alpha\beta} = \sum_{i} C^{m_\alpha}_{j_\alpha i} C^{m_\beta}_{j_\beta i} \frac{v_i}{u_i} \delta_{m_\alpha, -m_\beta} \qquad (III.7.4)$$

We could write this because when the exponential is expanded in a power series the extra terms vanish identically. We have denoted, here, the quantum numbers $(j_\alpha\ m_\alpha)$ by α and N is a normalisation constant.

The shell model hamiltonian is

$$H = \sum_{\alpha} \epsilon_\alpha a^{+}_{\alpha} a_\alpha + \frac{1}{4}\sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|V|\gamma\delta\rangle a^{+}_{\alpha} a^{+}_{\beta} a_\gamma a_\delta \qquad (III.7.5)$$

So, we can write the energy of a state with angular momentum J in the ground state rotational band as (c.f. eq. (II.2.10)

$$E_J = \frac{\langle\phi_0|H P^J_{00}|\phi_0\rangle}{\langle\phi_0|P^J_{00}|\phi_0\rangle}$$

$$= \frac{\int_0^{\pi/2} h(\theta) d^J_{00}(\theta) \sin\theta d\theta}{\int_0^{\pi/2} n(\theta) d^J_{00}(\theta) \sin\theta d\theta} \qquad \ldots (III.7.6)$$

The overlap integrals $h(\theta)$ and $n(\theta)$ are given by

$$h(\theta) = n(\theta)\left[\sum_{\alpha}\epsilon_{\alpha}\left(\frac{M}{1+M}\right)_{\alpha\alpha} + \frac{1}{4}\sum_{\alpha\beta\gamma\varepsilon}\langle\alpha\beta|v|\gamma\varepsilon\rangle \times \right.$$
$$\left. \times\left\{2\left(\frac{M}{1+M}\right)_{\gamma\alpha}\left(\frac{M}{1+M}\right)_{\varepsilon\beta} + \sum_{\mu}\left(\frac{1}{1+M}\right)_{\mu\varepsilon}\left(\frac{1}{1+M}\right)_{\gamma\beta}\right\}\right] \qquad \text{(III 7.7)}$$

and $$n(\theta) = \sqrt{det\left(1+M(\theta)\right)} \qquad \text{(III.7.8)}$$

respectively.

Here,

$$f_{\alpha\beta}(\theta) = \sum_{m'_{\alpha} m'_{\beta}} d^{j_{\alpha}}_{m_{\alpha} m'_{\alpha}}(\theta)\, d^{j_{\beta}}_{m_{\beta} m'_{\beta}}(\theta)\, f_{j_{\alpha} m'_{\alpha}, j_{\beta} m'_{\beta}} \qquad \text{(III.7.9)}$$

and, $$M = F f^{\dagger} \qquad \text{(III 7.10)}$$

The computation goes as follows. First by carrying out HFB calculation we get the intrinsic state $|\phi_0\rangle$ from this we set up the f-matrix. Then we compute the capital F matrix. This is done by the subroutine CAPF. The M-matrix is computed by the subroutine FSMF. 1/1+M and M/1+M (i.e. $1-(1+M)^{-1}$) are computed by the subroutine MATINV. Then the overlap integrals $h(\theta)$ and $n(\theta)$ are computed by the subroutine TBM. Finally we get E_J from the expression (III.7.6).

CHAPTER IV

RESULTS AND DISCUSSIONS

IV.1 1s-0d Shell:-

The 1s-0d has, since long, been considered a region of well-deformed nuclei. As pointed out by Ripka[1], one can associate well defined intrinsic states with the 1s-0d shell nuclei.

The 1s-0d shell nuclei have been extensively studied in the frame work of the exact shell model in the recent past[2]. It is thus not necessary to examine these nuclei in the framework of the phenomenological models such as IBM.

But, here we have found that the collective nature of the low-lying levels in the 1s-0d shell nuclei do indeed depend selectively on the V(J=0+2) part of the interaction. From Figs. (1-5) we have presented the low-lying collective levels of nuclei (^{22}Ne, ^{24}Ne, ^{24}Mg, ^{26}Mg, ^{30}Si) with J=0+2 interactions only, as well as full interactions so that the two spectra can be readily compared. Since we are mainly interested in the two-body part of the interaction, here and elsewhere, we have suppressed the role of single particle energies by making them degenerate i.e. making all of them zero.

IV.2 1p-0f Shell:-

To show that the emergence of the rotational spectra in the presence of the V(J=0+2) interaction (with the single particle energies absent) is not an attribute of our calculational framework, but an intrinsic property of the effective interactions (for the 1s-0d shell), we next present some results for the 1p-0f shell nuclei. The spectra resulting from the V(J=0+2) interaction in the case of the nuclei ^{50}Ti, ^{56}Fe, and ^{64}Ni exhibit a complete lack of rotational spectra (Figs. 6-8).

We may thus conclude that the IBM is likely to prove extremely poor phenomenological method for studying the low-lying levels in the A=40-70 mass range.

IV.3 0f-1p-0g Shell:-

In Figs. 9-10 we present the results for the nuclei ^{76}Kr and ^{78}Se in the 0f-1p-0g shell.

The results indicate that the qualitative features-the approximate J(J+1) behaviour-are unaffected in going from the full interaction to just its "J=0+2 subset, when the single particle energies are assumed to be degenerate.

We have also done the calculations for the nucleus ^{80}Kr (Fig.11). Here we find that the spectrum obtained with the V(J=0+2) interaction is no longer rotational for J $\geq$ 4. This feature may be related to the fact that the nucleus ^{80}Kr is the least deformed of the three nuclei.

considered by us in this region, because of the approaching shell closure at (Z=40,N=50).

It should be mentioned here that the spectra in 0f-1p-0g shell nuclei have actually been analysed in a phenomenological manner, with the help of the Interacting Boson Model. This work has been reported by Gelberg and U.Kaup[3] recently.

^{22}Ne

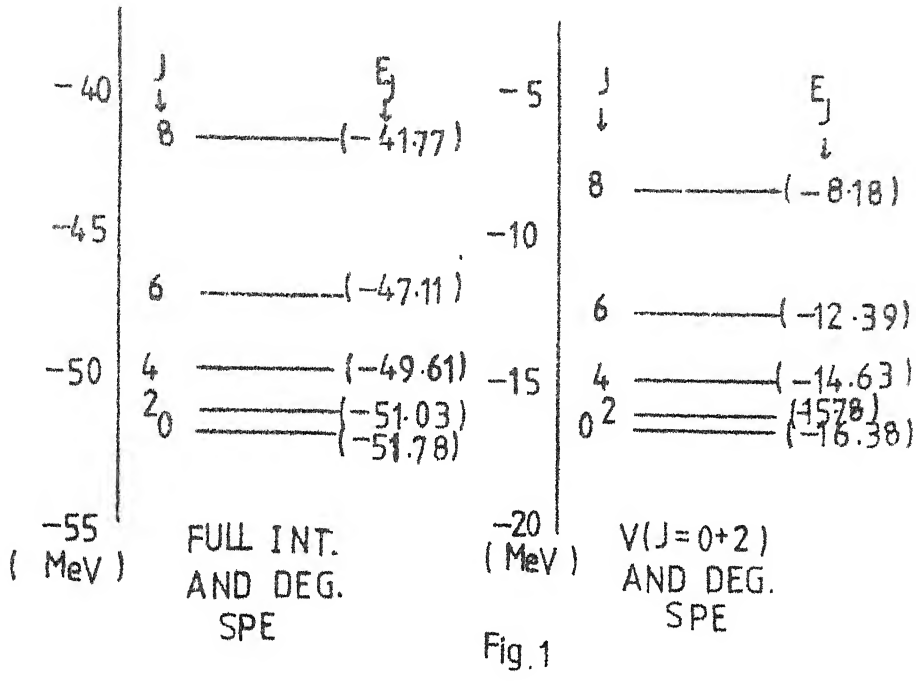


Fig. 1

^{24}Ne

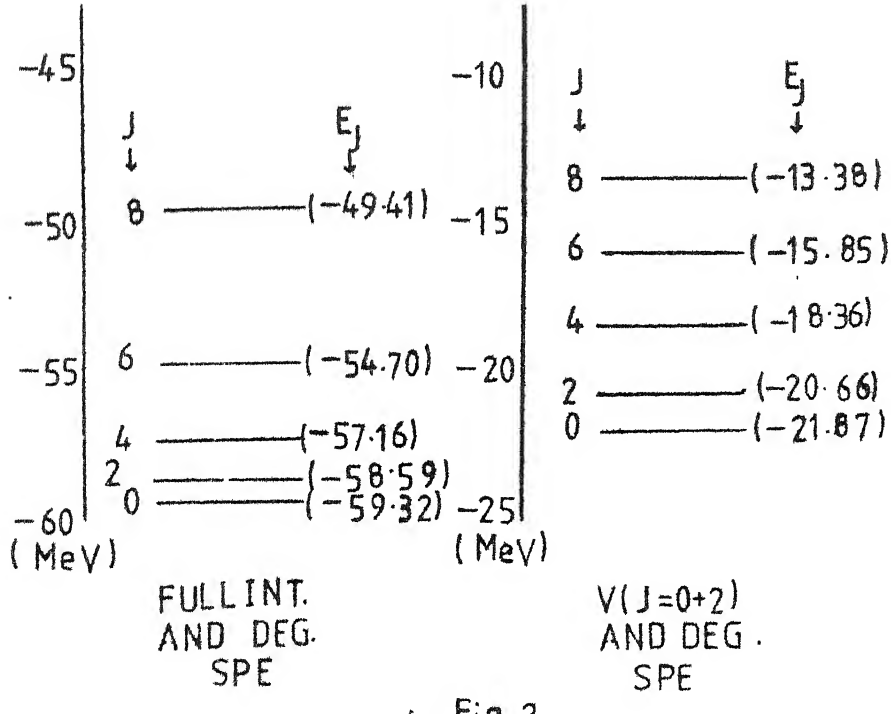


Fig. 2

^{24}Mg

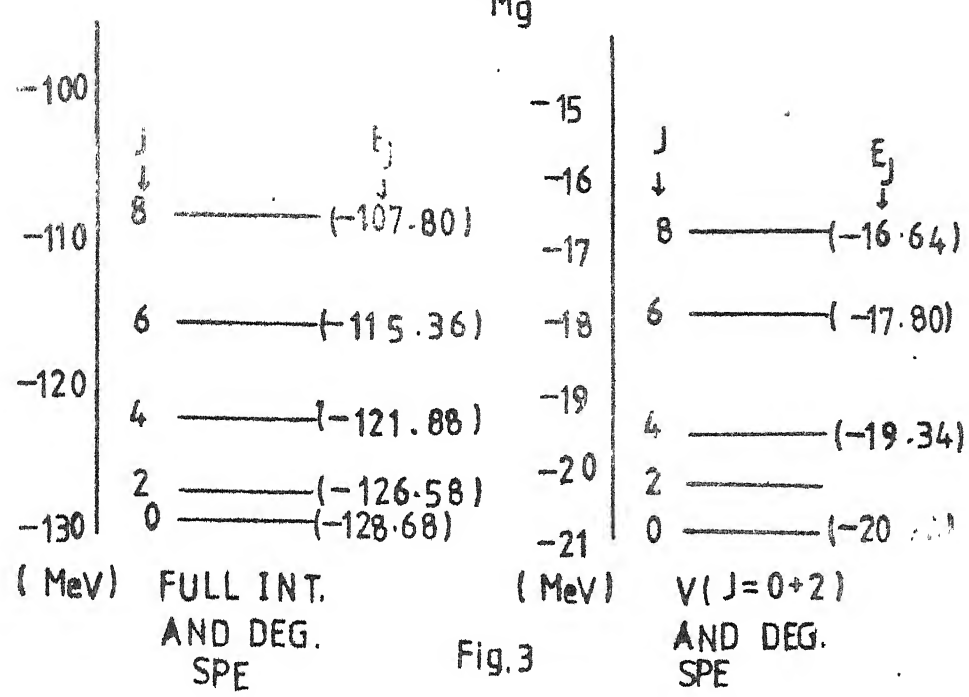


Fig.3

^{26}Mg.

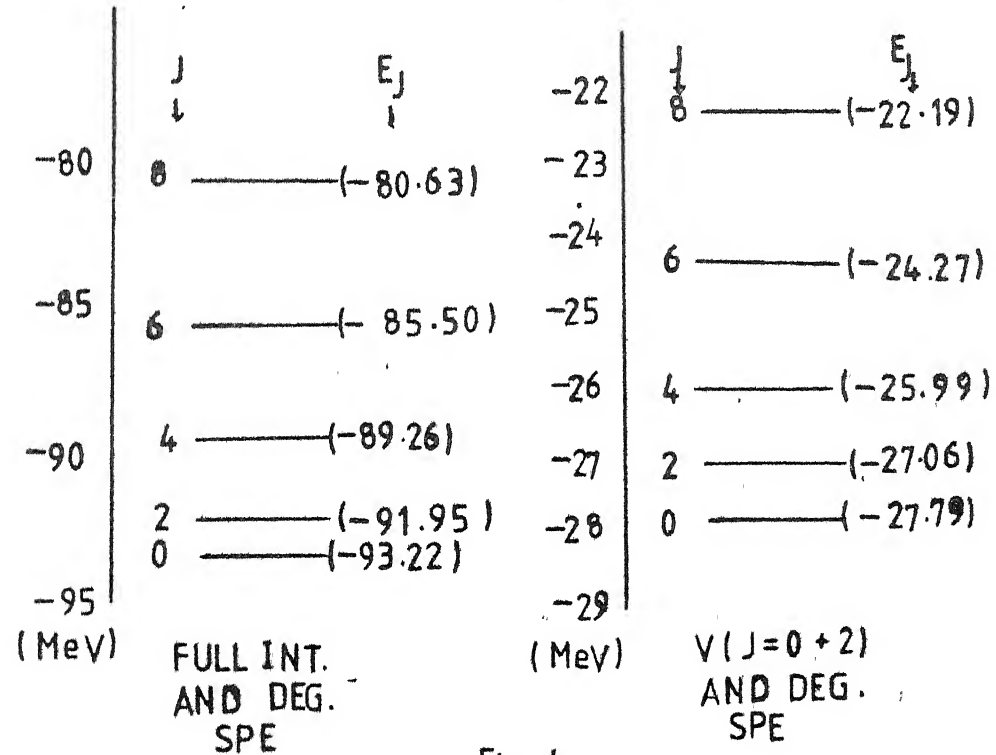


Fig.4

^{30}Si

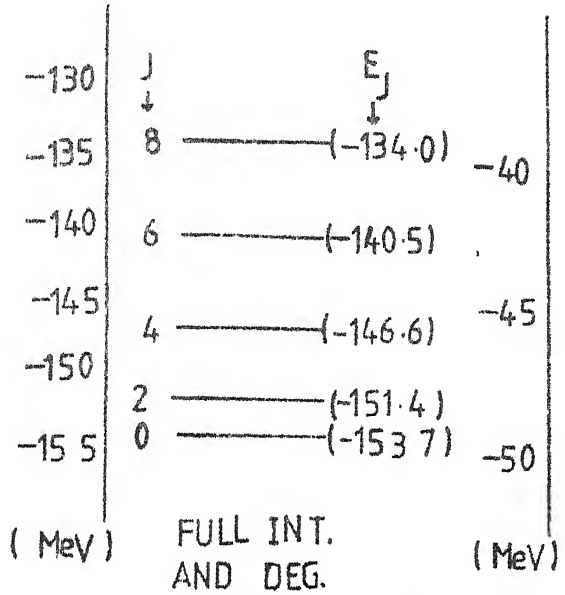


Fig. 5

^{50}Ti

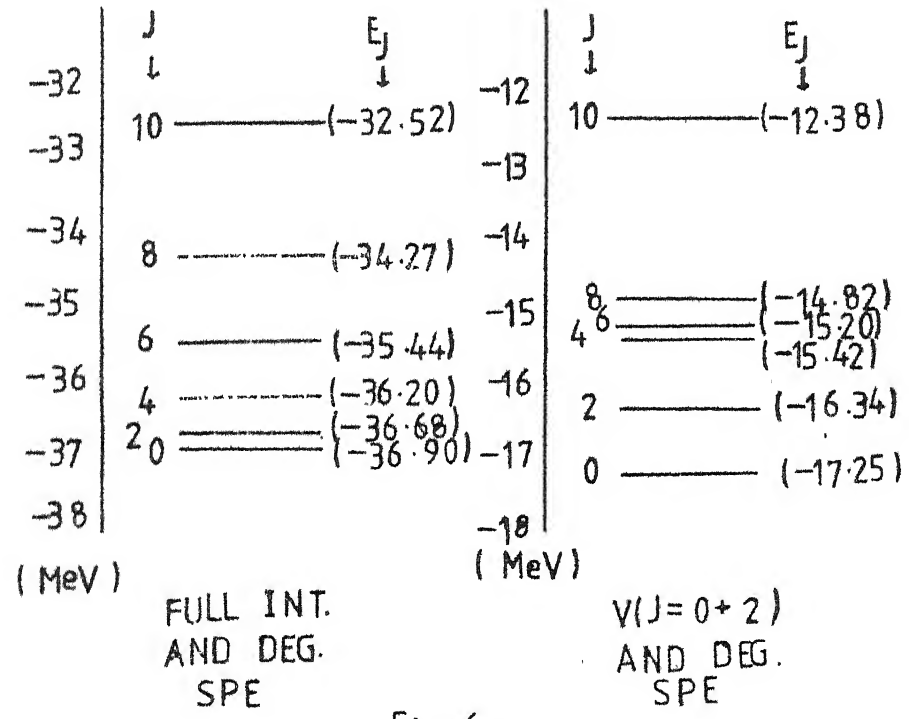


Fig. 6

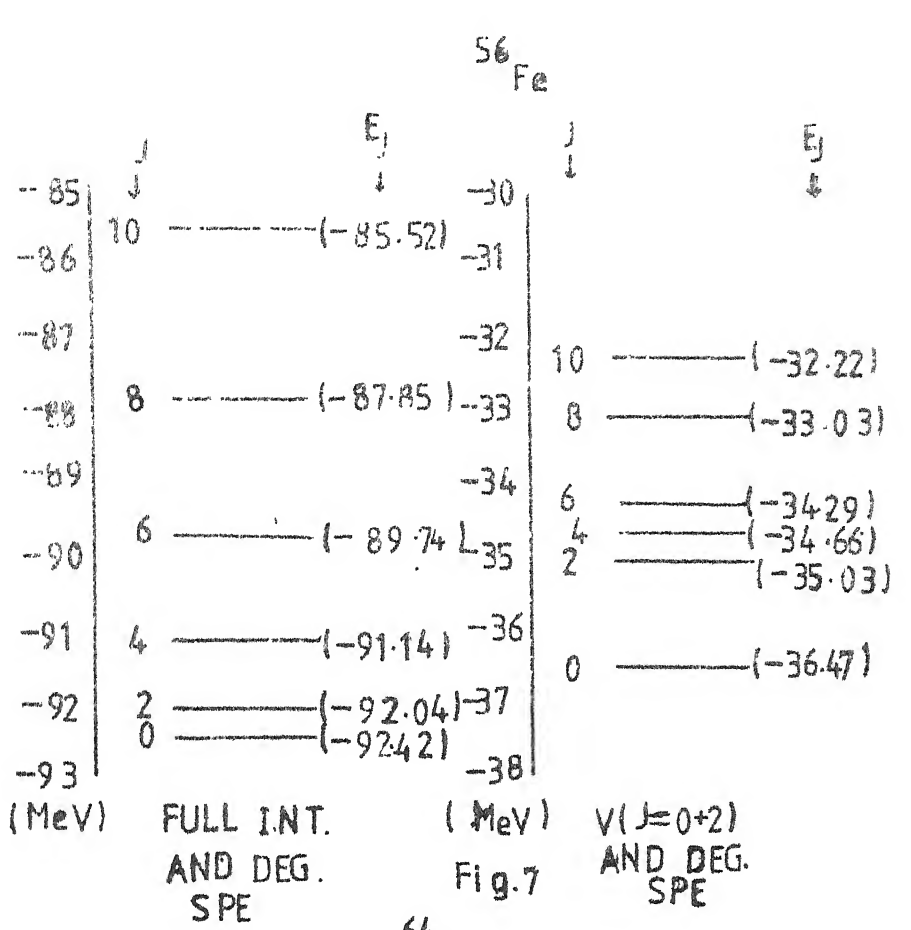
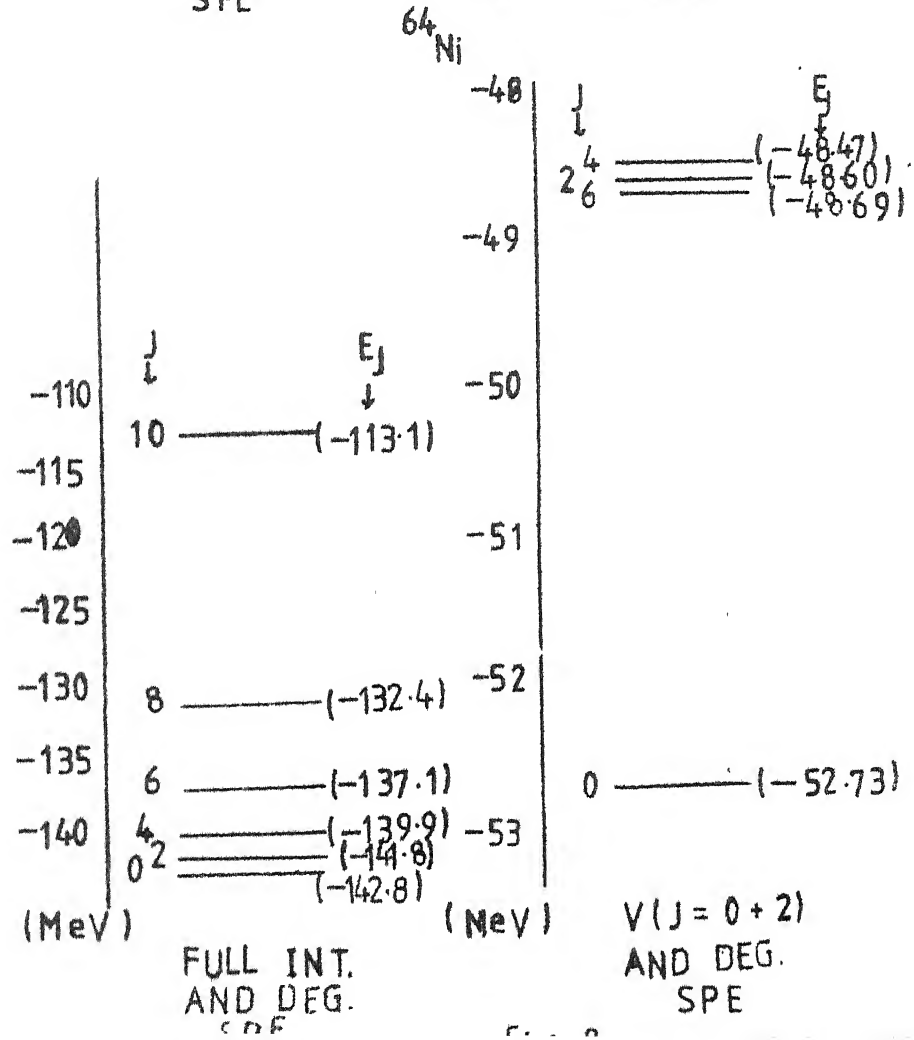

56Fe
J
Ej
10
(-85.52)
8
(-87.85)
6
(-89.74)
4
(-91.14)
2
(-92.04)
0
(-92.42)
-85
-86
-87
-88
-89
-90
-91
-92
-93
(MeV)
FULL I.NT.
AND DEG.
SPE
-30
-31
-32
-33
-34
-35
-36
-37
-38
(MeV)
10
(-32.22)
8
(-33.03)
6
(-34.29)
4
(-34.66)
2
(-35.03)
0
(-36.47)
V(J=0+2)
AND DEG.
SPE

Fig.7


64Ni
-48
-49
-50
-51
-52
-53
4
6
(-48.47)
(-48.60)
(-48.69)
10
(-113.1)
8
(-132.4)
6
(-137.1)
4
2
0
(-139.9)
(-141.8)
(-142.8)
-110
-115
-120
-125
-130
-135
-140
(MeV)
FULL INT.
AND DEG.
SPE
(MeV)
0
(-52.73)
V(J = 0 + 2)
AND DEG.
SPE

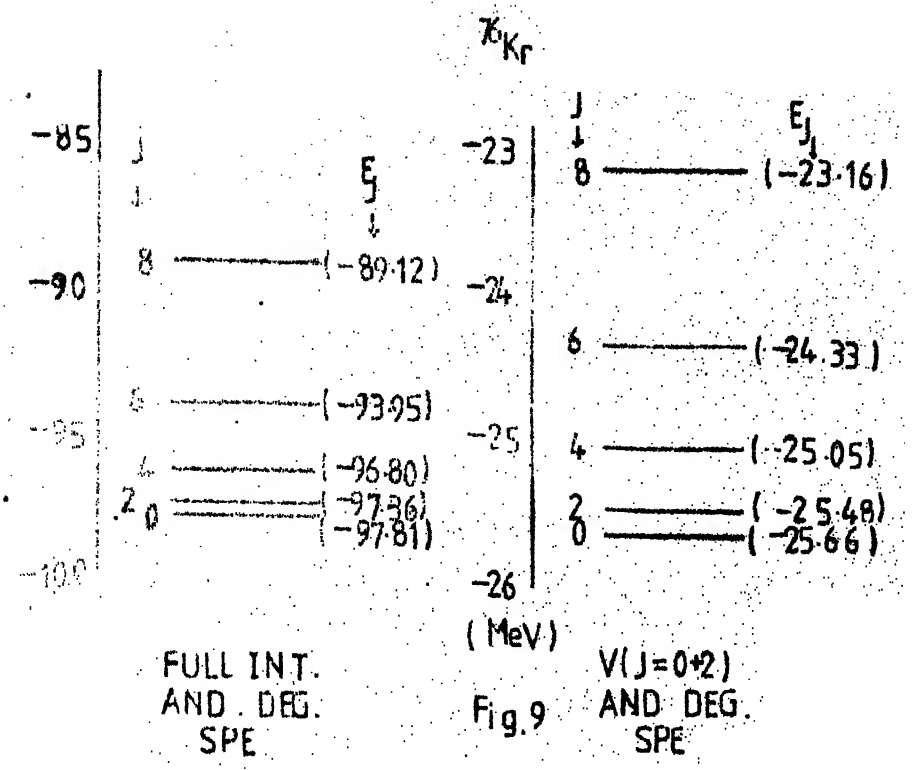

^{76}Kr
-85
-90
-95
-100
J
E
8 (-89·12)
6 (-93·95)
4 (-96·80)
2 (-97·36)
0 (-97·81)
-23
-24
-25
-26
(MeV)
J
E
8 (-23·16)
6 (-24·33)
4 (-25·05)
2 (-25·48)
0 (-25·66)
FULL INT. AND DEG. SPE
V(J=0+2) AND DEG. SPE

Fig. 9

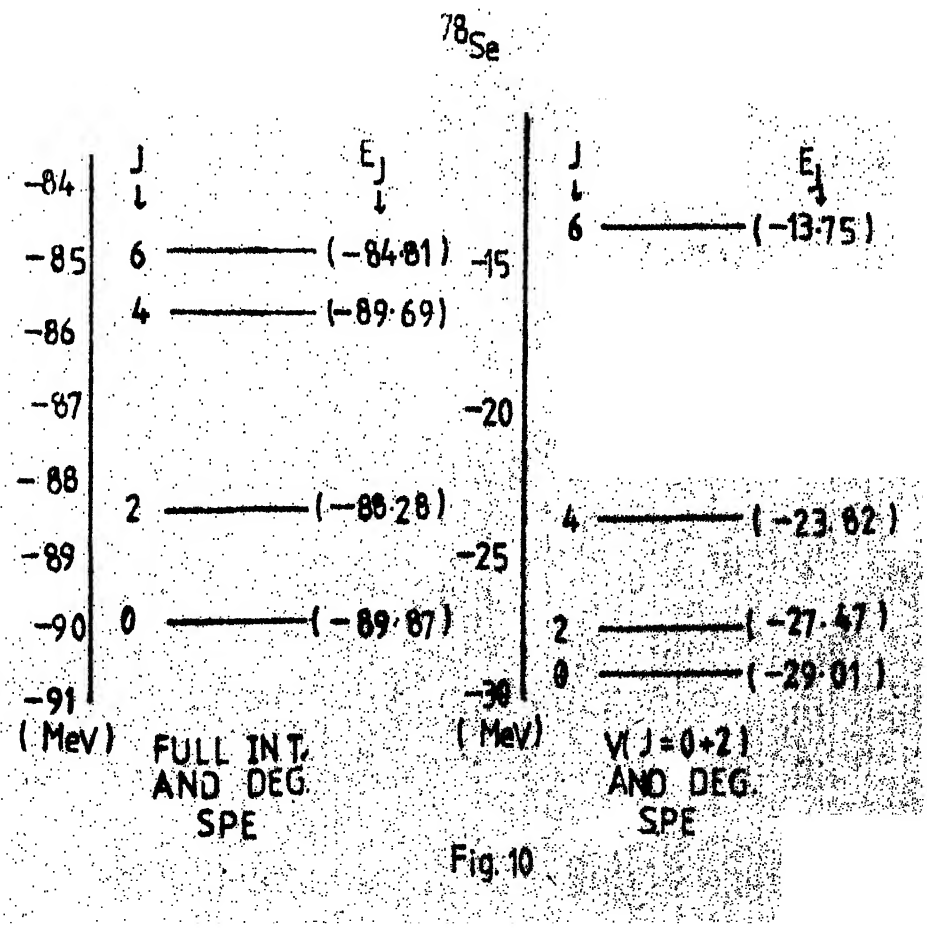

^{78}Se
-84
-85
-86
-87
-88
-89
-90
-91
(MeV)
J
E
6 (-84·81)
4 (-89·69)
2 (-88·28)
0 (-89·87)
-15
-20
-25
-30
(MeV)
J
E
6 (-13·75)
4 (-23·82)
2 (-27·47)
0 (-29·01)
FULL INT. AND DEG. SPE
V(J=0+2) AND DEG. SPE

Fig. 10

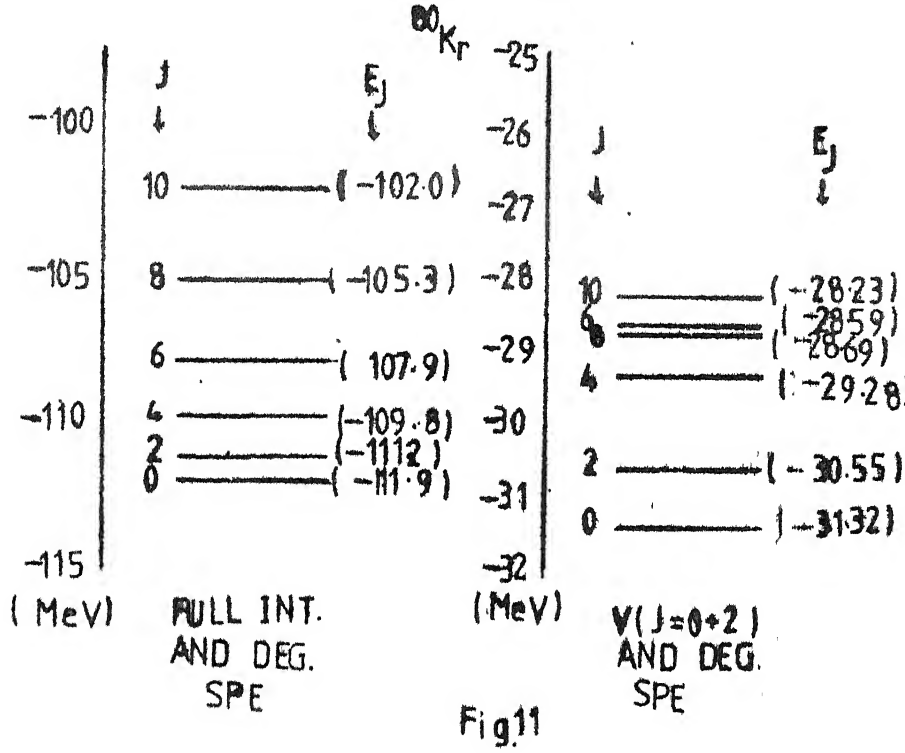

80Kr
J
Ej
10
8
6
4
2
0
(-102·0)
(-105·3)
(-107·9)
(-109·8)
(-111·2)
(-111·9)
-100
-105
-110
-115
(MeV)
FULL INT.
AND DEG.
SPE
-25
-26
-27
-28
-29
-30
-31
-32
(MeV)
J
Ej
10
8
6
4
2
0
(-28·23)
(-28·59)
(-28·69)
(-29·28)
(-30·55)
(-31·32)
V(J=0+2)
AND DEG.
SPE

Fig.11

CHAPTER V

CONCLUSION

In 1s-0d and 0f-1p-0g shell nuclei, the structure of the low-lying collective levels depends selectively only on the J=0 and J=2 nucleon pairs. In 0f-1p shell nuclei, the low-lying collective spectra are not reproduced when one employs the effective interaction operating only in the J=0 and J=2 states.

Since the selective dependence of the collective features on only the J=0,2 subset of interaction is an important ingradient of the Interacting Boson Model, one can infer that the model is likely to be more successful in the 1s-0d and 0f-1p-0g shells than in the 0f-1p shell.

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